Predicting Chemical and Physical Properties and Reactivity for Industrial Applications

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Conventional experimental measurements are unable to keep up with the increasing property data needs of industry. Discovery and process optimization are limited by a lack of property data and insight into mechanisms that determine performance. For the vast majority of applications, particularly those involving mixtures and complex systems, evaluated property data simply do not exist and are difficult, time-consuming, or expensive to obtain. Theoretical and computational methods have the potential to meet much of this need by supplementing experiment and providing data in a timely manner at lower cost. For the vast majority of industrial applications, however, currently available computational methods are limited by a lack of flexibility and validation, i.e. the quality of predicted properties is generally unknown, particularly for novel systems. Models based exclusively on first principles are highly accurate, flexible and extensible, but can only be applied to very small systems and must be "coarse-grained" (approximated by averaging over larger regions) for the time and length scales required in industrial applications. In this presentation we will highlight current efforts of the NIST Computational Chemistry group to develop and validate theoretical and computational methods to predict chemical and physical properties, reactivity, and rate constants with quantitative measures of uncertainty. Approaches for integrating theoretical predictions with evaluated experimental data and knowledge-based software guides to deliver data on demand will be presented.